Solution-Processable Septithiophene Monolayer Transistor

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Supporting Information

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Supporting Information

Table S1. Experimental and calculated d-spacings of the triclinic unit cell of 7T studied at room temperature.

h	k	l	d_{exp}, Å	d_{calc}, Å
1	0	0	34.33	34.44
2	0	0	17.06	17.22
3	0	0	11.38	11.48
4	0	0	8.57	8.61
5	0	0	6.87	6.89
6	0	0	5.75	5.74
7	0	0	4.94	4.92
8	0	0	4.34	4.31
9	0	0	3.80	3.83
10	0	0	3.47	3.44
2	1	0	8.74	8.75
0	1	0	8.45	8.45
3	1	0	8.12	8.13
1	-1	0	7.67	7.67
4	1	0	7.31	7.28
2	-1	0	6.80	6.79
3	-1	0	6.00	5.97
4	-1	0	5.27	5.26
7	1	0	5.00	4.99
5	-1	0	4.68	4.67
6	-1	0	4.20	4.18
7	-1	0	3.80	3.77
8	-1	0	3.47	3.43
9	-1	0	3.19	3.14
0	0	2	5.66	5.68
3	0	-2	4.71	4.70
7	0	-2	3.41	3.40
1	2	0	4.39	4.41
4	1	2	4.26	4.24
1	-2	1	4.10	4.11
3	-2	1	3.91	3.92

Table S2 Experimental and calculated d-spacings of the triclinic unit cell of 7T measured at 100°C

h	k	l	d_{exp}, Å	d_{calc}, Å
1	0	0	32.19	32.05
2	0	0	15.83	16.02
3	0	0	10.56	10.68
4	0	0	7.95	8.01
5	0	0	6.39	6.41
6	0	0	5.35	5.34
7	0	0	4.62	4.58
8	0	0	4.07	4.01
5	-1	0	4.63	4.63
6	-1	0	4.12	4.13
7	-1	0	3.71	3.71
8	-1	0	3.37	3.36
0	0	2	5.88	5.87
2	0	2	5.63	5.60
-1	0	2	5.72	5.72
-2	0	2	5.47	5.42
3	0	2	5.19	5.25
4	0	2	4.83	4.85
5	0	2	4.45	4.44
6	0	2	4.09	4.05
-4	1	2	3.84	3.83
-5	1	2	3.56	3.57
-6	1	2	3.31	3.31
-7	1	2	3.07	3.08
-3	0	2	4.99	5.04
-5	0	2	4.22	4.22

For reconstruction of the profile ten orders of the 100 peak were used. The electron density profile (EDP) was computed using Lorentz-corrected intensities of h00 peaks I_n as following:

$$E(r) = \sum_{n=0}^{N} A_n \cos\left(\frac{2\pi n\, r}{c} + \varphi_n\right),$$

where $A_n=(I_n)^{1/2}$ is the amplitude of the n^{th} diffraction order peak, c -the periodicity in the **a***-direction and φ_n - the phase. The values of the phase (in this centro-symmetric structure the phase equals either 0 or π) was established based on the comparison of the EDF calculated from the experimental intensities of the h00 peaks for different sets of phases with the EDF

profile calculated from our structural model. Only the phases of the most intense peaks such as 100, 200, 400, 600, 800 have been varied, whereas the phases of the other peaks were set to 0. The best coincidence was found for the case where for 400 and 600 reflexes the phase is equal to π and for other peaks the phase was set to zero (Figure 1b-c). On the profile high-density regions (23.2 Å) corresponding to thiophene layers alternate with low-density layers of alkyl chains (11.2 Å). The found layer thickness is in a good agreement with X-ray reflectivity data.

Optical spectroscopy:

The fluorescence and excitation spectra of the fully covered 7T monolayer measured at low temperature (80 K) are shown in Figure S1. The film obtained with 0.9 g/l, corresponding to 100% coverage, shows the onset of fluorescence at 2.1 eV with a maximum intensity at about 1.9 eV. The excitation spectrum shows an onset at 2.27 eV with a maximum intensity near 2.4 eV. The fluorescent excitation has a similar pattern as room temperature excitation. However, the fluorescent spectra of the films are different respect to the room temperature spectra. The energy position of the peaks at low temperature is unchanged but the intensity of the transition decreases and new bands appear at low temperature. This can be interpreted as temperature induced reorganization. At low temperature there is mainly emission from species that give rise to the new peaks.

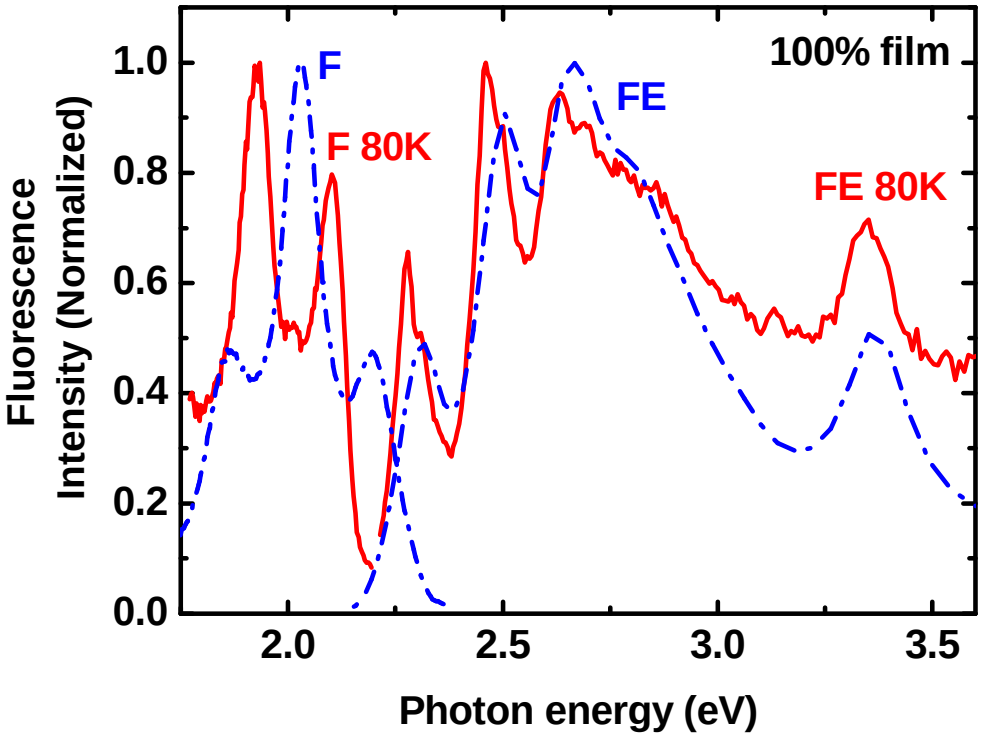

Figure S1. Fluorescence (F) and fluorescent excitation (FE) spectra of a fully covered sample (0.9 g/L = 100% film) of 7T molecules on quartz, measured at 80K.